Data Evaluation Record on the anaerobic biotransformation of chloropicrin in water-sediment system

PMRA Submission Number {.....} EPA MRID Number 43759301

Data Requirement: PMRA Data Code:
EPA DP Barcode: D314391
OECD Data Point:
EPA Guideline: 162-3

Test material:
Common name: Chloropicrin.
Chemical name:
IUPAC name: Trichloronitromethane.
CAS name: Trichloronitromethane.
CAS No: 76-06-2.
Synonyms:
SMILES string: O=N(=O)C(Cl)(Cl)Cl (EPI Suite, v3.12 SMILES).

Primary Reviewer: Dana Worcester
Cambridge Environmental
Signature: Dana Worcester
Date: 05/16/07

Secondary Reviewer: Joan Gaidos
Cambridge Environmental
Signature:
Date: 05/16/07

QC/QA Manager: Joan Gaidos
Cambridge Environmental
Signature:
Date: 05/16/07

Final Reviewer: Faruque Khan
EPA Reviewer
Signature:
Date: 3/14/08

Company Code:
Active Code:
Use Site Category:
EPA PC Code: 081501

CITATION: Hatton, C., K. Shepler and L. Ruzo. 1995. Anaerobic aquatic metabolism of [^{14}C]chloropicrin. Unpublished study performed by PTRL West, Inc., Richmond, California; sponsored and submitted by Chloropicrin Manufacturers Task Force, c/o Niklor Chemical Company, Long Beach, California. PTRL Report No.: 449W-1 and Project No.: 449W. Experimental start and completion date and final report date were not available.

Data Evaluation Record on the anaerobic biotransformation of chloropicrin in water-sediment system

PMRA Submission Number {.....} EPA MRID Number 43759301

EXECUTIVE SUMMARY

The biotransformation of [^{14}C]-labeled trichloronitromethane (chloropicrin; radiochemical purity >99.9%) was studied in nitrogenated, deionized water-sandy loam soil (water pH 7.7; sediment pH 7.2, organic matter 1.3%) systems from California for 54 days under anaerobic (static, nitrogen atmosphere) conditions in darkness at 25 ± 1°C. [^{14}C]Chloropicrin was applied at a rate of *ca.* 300 mg a.i./L. The soil:water ratio used was 1:4.4 (20 g sediment:87 mL water). The guideline and GLP Standards were not reported. The test system consisted of biometer flasks with a sidearm containing 10% KOH and polyurethane foam. To generate anaerobic conditions, the water-soil systems were purged with nitrogen, then the sealed flasks were pre-incubated for 4 weeks prior to treatment. Following treatment, duplicate flasks were collected after 1.5 hours, 1, 2, 5, 12, 26 and 54 days of incubation. Additional samples (designated as "supplemental samples") were prepared and incubated as described and analyzed at 0 and 4 hours posttreatment. Aliquots of the headspace were analyzed by LSC following combustion and the 1.5 hour aliquot was injected into acetonitrile and analyzed by HPLC. Water layers were analyzed by LSC and HPLC without modification or manipulation. Soil samples were extracted three times with acetonitrile. Resulting sediment extracts were combined and analyzed by HPLC analysis. Identifications were confirmed by a second HPLC method. Samples were cochromatographed with nitromethane, sodium bicarbonate, methanol, 1,3,5-trioxane, 2-nitrophenol and formaldehyde.

The test conditions outlined in the study appear to have been maintained throughout the 54-day incubation. The systems were moderately reducing with redox potentials of -10 to +198 mV. In the water layer, dissolved oxygen was 0.23-1.63 (units not reported); pH levels were 6.6-7.9, with the exception of 8.1-8.7 at days 2 and 54 (one of two replicates).

Overall recovery of radiolabeled material averaged 98.2 ± 2.8% (range 91.4-103.0%) of the applied, with no pattern of decline in recoveries during the 54-day study. Following application of [^{14}C]chloropicrin to the water-soil systems, [^{14}C]residues partitioned from the water layer to the soil with average (n = 2) distribution soil:water ratios of 1:17 at time 0, 1:6 at 1 day, 1:1 at 12-26 days and was 2:1 at 54 days.

[^{14}C]Chloropicrin dissipated rapidly in the total system decreasing from 96.3% (one replicate) of the applied at time 0 to an average of 45.5% at 1.5 hours (0.06 days) days to 1.1% at 2 days, was not detected from 5 to 12 days, and was last detected at 0.1% (one replicate) at 26 days posttreatment. In the water layer, [^{14}C]chloropicrin decreased from 91.7% at day 0 to 26.7% at 1.5 hours (0.06 days) days to 0.6% at 2 days, was not detected from 5 to 12 days, and was last detected at 0.1% (one replicate) at 26 days posttreatment. In the soil, [^{14}C]chloropicrin was detected in a single replicate; 4.6% of the applied at time 0. Observed DT50 values of chloropicrin were <1.5 hours in the water layer and total system. Based on first order linear regression, the half-lives of chloropicrin were 0.4 days in the water layer and total system. Based on nonlinear analysis (SigmaPlot v 9), half-lives were 0.03 days in the water and total system. A half-life in soil could not be calculated because it was detected in a single replicate at time 0.

Two major transformation products were isolated and no minor products were identified. Nitromethane increased to maximum average of 57.4% (53.4% in water, 3.3% in soil) of the applied at 1 day and was last detected at 16.9% (one replicate) at 26 days. Chloronitromethane increased to a maximum average of 53.1% (51.5% in water, 1.6% in soil) of the applied at 4 hours (0.17 days) and was <0.2% thereafter. Unidentified polar [^{14}C]residues were detected at maximum averages of 13.0%, 0.6%, 13.0% and 0.3% of the applied in the water, soil, total system and volatiles, respectively. An unknown with an Rt of 9 minutes was a maximum 7.3%, 0.7% and 8.0% of the applied in the water layer, soil and total system, respectively. Extractable soil [^{14}C]residues were 4.1-4.3% of the applied at 0-1 day and were 1.3-2.9% thereafter. Nonextractable soil [^{14}C]residues increased from 1.2% of applied at time 0 to 32.0% at 54 days. At study termination, organic matter fractionation of nonextractable [^{14}C]residues found 24.4% and 1.3% of the applied radioactivity associated with the fulvic acids and humic acids, respectively.

Results Synopsis:

Test system used: Deionized water-sandy loam soil California.

Linear half-life in water:	0.4 days (r^2 = 0.5609).
Linear half-life in sediment:	ND (not determined).
Linear half-life in the total system:	0.4 days (r^2 = 0.559).
Non-linear half-life in water:	0.03 days (r^2 = 0.9972).
Non-linear half-life in sediment:	ND.
Non-linear half-life in total system:	0.03 days (r^2 = 0.9973).
Observed DT50 in water:	<1.5 hours.
Observed DT50 in sediment:	ND.
Observed DT50 in total system:	<1.5 hours.

Major transformation products:
Nitromethane.
Chloronitromethane.
Minor identified transformation products:
CO_2.

The Chloropicrin Manufacturers' Task Force submitted comments to EPA regarding the Phase 3 Risk Assessment for Chloropicrin. In these comments, the Task Force cites that EPA calculated an anaerobic aquatic metabolism half-life of 0.05 days (methods not described) for chloropicrin (p. 29 of *Comments on USEPA's Chloropicrin Risk Assessment Phase 3,* February 28, 2007; FRL: 8087-4; EPA-HQ-OPP-2006-0661).

In reformatting the original DER into the current harmonized templates used by EPA, the current reviewer calculated the anaerobic aquatic metabolism half-life for chloropicrin using the data provided in the original DER and the current EFED methods using all data points: first-order linear

regression using Excel 2000, and single, two-parameter exponential decay non-linear regression using SigmaPlot v. 9. The current reviewer obtained a total system linear half-life of 0.4 days (9.6 hours) and a non-linear half-life of 0.03 days (0.7 hours); the study author calculated DT50 was 0.05 days (1.3 hours), and the observed DT50 was <0.06 days (<1.5 hours).

Study Acceptability: This study is classified as **acceptable**. No significant deviations from good scientific practices were noted.

EPA indicated that this study did not meet Subdivision N Guidelines due to two problems: The test water was not representative of the intended use site (purified deionized water was utilized to flood the soil samples); and the analytical methods were inadequate for the characterization of the residues in water samples removed at later sampling intervals (low column recoveries in the HPLC analysis). The Chloropicrin Manufacturers' Task Force responded to these two problems (p. 38 of *Comments on USEPA's Chloropicrin Risk Assessment Phase 3,* February 28, 2007; FRL: 8087-4; EPA-HQ-OPP-2006-0661):

- Because chloropicrin has no aquatic uses, the primary mode of interaction with water will be chloropicrin in/on soil exposed to rainwater. Therefore, soil from a growing region and deionized water were used, rather than sediment and natural water. Suitability of the test system was characterized throughout the study by measuring pH, Eh, and dissolved oxygen.

- The analytical methods were consistently successful in identifying and quantitating a variety of volatile, water soluble species isolated from aqueous and soil matrices. Loss of material from water column recoveries was ascribed to the formation of methanol as a degradate, which is a volatile material and probably accounts for these low recoveries.

I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study guidelines were not cited. No significant deviations from the objectives of Subdivision N guidelines were noted.

COMPLIANCE: This study GLP Standards were not cited. The signed and dated Data Confidentiality, GLP, Quality Assurance and [study] Certification statements were not provided.

A. MATERIALS:

1. Test Material [^{14}C]Chloropicrin (p. 18; Figure 1, p. 61).

Chemical Structure: See DER Attachment 1.

Description: Not reported.

Purity:

Radiochemical purity:	>99.9% (p. 18; Figure 1, p. 61).
Lot/Batch No.	Not reported.
Analytical purity:	Not reported.
Specific activity:	1.1 mCi/mmol.
Location of the radiolabel:	Not reported.

Storage conditions of test chemicals: Not reported.

Physico-chemical properties of chloropicrin:

Parameter	Value	Comment
Water Solubility	Not reported.	
Vapor Pressure	Not reported.	
pK_a	Not reported.	
K_{ow}	Not reported.	
Stability of compound at room temperature	Not reported.	

2. Water-sediment collection, storage and properties

Table 1: Description of water-sediment collection and storage.

Description		Details
Geographic location.		Watsonville, California.
Pesticide use history at the collection sites		Not reported.
Collection date		Not reported.
Collection procedures for:	Water:	Nitrogenated, deionized water.
	Soil:	Not reported.
Sampling depth for:	Water:	Not applicable.
	Soil:	Not reported.
Storage conditions		Not reported.
Storage length		Not reported.
Preparation	Water:	Not reported.
	Soil:	Seived (2 mm).

Data obtained from pp. 25-26 of the study report.

Table 2: Properties of the water.

Property	**Details**	
Temperature (°C)	Not reported.	
Not reported.	7.7	
Redox potential (mV)	Initial[1]	Final
	+133-157	+112-136
Oxygen concentration (units not reported)	Initial[1]	Final
	0.37-2.64	0.32-0.45
Dissolved organic carbon (mg/L)	Not reported.	
Hardness (mg $CaCO_3$/L)	2	
Electrical conductivity (µmho/cm)	0	
Biomass (cells/mL water)	Not reported.	

1 Initial values were the supplemental time 0 sample values.
Data obtained from pp. 25-26; Table VII, p. 53 of the study report.

Table 3: Properties of the soil.

Property	Details	
Soil texture	Sandy loam	
% Sand	53.2	
% Silt	27.2	
% Clay	19.6	
pH	7.2	
Organic carbon (%)[1]	0.7	
Organic matter (%)	1.27	
CEC (meq/100 g)	12.46	
Moisture at 15 bar (%)	8.56	
Moisture at 1/3 bar (%)	16.14	
Bulk density (g/cm^3)	1.12	
Biomass (system; CFU/g)	Initial	Final
	11.95×10^6	0.1725×10^6

1 Reviewer-calculated using the following equation: Organic carbon (%) = Organic matter (%)/1.72.
Data obtained from Table II-III, pp. 48-49 of the study report.

B. EXPERIMENTAL CONDITIONS:

1. Preliminary experiments: None reported.

2. Experimental conditions:

Table 4: Experimental design.

Parameter		Details
Duration of the test		54 days.
Water: Filtered/unfiltered water: Type and size of filter used, if any:		Nitrogenated, deionized.
Amount of sediment and water per treatment	Water:	87 mL.
	Sediment:	20 g dry wt.
Water/sediment ratio		4.4:1 (mL:g).
Application rates (mg a.i./L)	Nominal:	*ca.* 300 mg a.i./L (313 ± 14.4 µg a.i./g)
	Actual:	269 to 303 mg a.i./L
Control conditions, if used		No sterile controls were used.
No. of replications	Control, if used:	No sterile controls were used.
	Treated:	Enough flasks were prepared to allow for duplicate flasks at each sampling interval.
Test apparatus (type/material/volume):		Biometer flasks with a sidearm flask for the collection of volatiles. An illustration of the test apparatus is provided in

Parameter		Details	
		Appendix A, p. 173 of the study report.	
Details of traps for CO_2 and organic volatile, if any:		The side arm flask contained 10% KOH and a polyurethane foam plug.	
If no traps were used, is the system closed?		Closed.	
Identity and concentration of co-solvent		Acetonitrile (ACN); final concentration not reported.	
Test material application method	Volume of the test solution used/treatment:	Not reported.	
	Application method (eg: mixed/not mixed):	Not reported.	
Any indication of the test material adsorbing to the walls of the test apparatus?		Not indicated.	
Microbial biomass/microbial population of controls (units)		Initial	Final
	Water:	No sterile controls were used.	
	Sediment:		
Microbial biomass/microbial population of treated (anaerobic CFU/g)		Initial	Final
	Sandy loam soil/water:	11.95×10^6	0.1725×10^6
Experimental conditions:	Temperature (°C):	25 ± 1°C; maintained in a temperature-controlled incubator.	
	Continuous darkness (Yes/No):	Yes; system flasks wrapped with aluminum foil and maintained in darkness in an incubator.	
Other details, if any		None	

Data obtained from pp. 19, 25-27; Table III, p. 49; Table V, p. 51; Appendix A, p. 173; Appendix E, pp. 196-197 of the study report.

3. Anaerobic conditions: Water-soil systems were prepared, purged with nitrogen (flow rate, interval not reported) and maintained in sealed biometer flasks for 4 weeks prior to treatment to establish anaerobic conditions (p. 27). Following treatment, the systems were maintained in a nitrogen atmosphere (Appendix E, pp. 196-197). At time 0 posttreatment in supplemental samples redox potential and dissolved oxygen in the water layer were +133-157 mV and 0.37-2.64 (units not reported), respectively (Table VII, p. 53).

An additional sample was prepared and treated with the oxygen indicator, resazurin (p. 28). The samples remained clear indicating that oxygen was not present (Appendix E, pp. 196-197).

4. Supplementary experiments: Because of the rapid degradation, additional supplemental samples were prepared and incubated as described for the definitive study (p. 21). The samples were collected at time 0 and 4 hours.

To determine of the KOH trapping solution reacted with chloropicrin, an aliquot of the stock solution was mixed with 10% KOH and treated with barium chloride (p. 29).

5. Sampling:

Table 5: Sampling details.

Criteria	Details
Sampling intervals	0, 0.06, 0.17, 1, 2, 5, 12, 26 and 54 days.
Sampling method	Duplicate treated systems at each interval.
Method of collection of CO_2 and organic volatile compounds	Volatile traps were collected at each sampling interval. Aliquots of the headspace were collected at each interval.
Sampling intervals/times for:	
Sterility check, if sterile controls are used:	Sterile controls were not prepared.
Redox potential, dissolved oxygen and pH in water layer and redox potential in sediment:	Measured at each sampling interval.
Sample storage before analysis	After separation, the water layer was stored frozen.
Other details, if any	None reported.

Data obtained from pp. 19, 28; Table IV, p. 50 of the study report.

C. ANALYTICAL METHODS:

Separation of the water and sediment: Aliquots of the water layer were removed for analysis (p. 28). Following removal of the water aliquots, the water:soil was centrifuged and the water decanted.

Extraction/clean up/concentration methods for water and sediment samples: The water layer was analyzed with modification or manipulation (pp. 28, 31).

The soil was extracted three times with acetonitrile via mechanical shaking (p. 29). The extract was separated from soil by centrifugation and was then decanted. The extracts were combined and analyzed by LSC and HPLC.

Total ^{14}C measurement: Total ^{14}C residues were determined by summing the concentrations of residues measured in the water layers, sediment extracts, extracted sediment, headspace and volatile trapping solutions (Table VI, p. 52).

Determination of nonextractable residues: Aliquots of the extracted soil were analyzed for total radioactivity by LSC following combustion (p. 29).

Organic matter fractionation. Aliquots of 2, 5, 12, 26 and 54-day extracted soil were further extracted two times with 0.5M sodium hydroxide, with the resulting extract separated from sediment by centrifugation (p. 29). The supernatant was decanted, analyzed for total radioactivity by LSC, then acidified to pH 1 with hydrochloric acid with the resulting precipitate (humic acids) removed by centrifugation. The resulting supernatant (fulvic acids) was analyzed for total radioactivity using LSC. [^{14}C]Residues remaining in the precipitate (humic acids) was redissolved in 0.5M NaOH and analyzed using LSC.

Determination of volatile residues: Triplicate aliquots of the KOH trapping solutions were analyzed for total radioactivity by LSC (p. 28). The identification of CO_2 was confirmed using precipitation with barium chloride (p. 29). The day 2 aqueous phase was incubated overnight with 10% KOH and analyzed by HPLC (p. 42). The polyurethane foam plugs were soaked overnight in acetonitrile and aliquots were analyzed by LSC.

Aliquots of the headspace from each sampling interval were analyzed by LSC (p. 28). An aliquot from 1.5 hour (0.06 days) was injected into acetonitrile and analyzed by HPLC.

Derivatization method, if used: None was reported.

Identification and quantification of parent compound: Water and soil extract samples were analyzed by HPLC under the following conditions: LC 18 column, gradient mobile phase of water:acetonitrile starting at 100:0 and ending at 0:100, UV detector (220 nm), and radioactivity detector (p. 31).

To confirm results from HPLC Method I, a select sample (day 2) was also analyzed by HPLC under the following conditions: Amines Ion Exclusion HPX-87H column, isocratic mobile phase using 0.01N H_2SO_4, refractive index detection (pp. 31, 40). To identify the radioactivity in the traps, the aqueous phase from day 2 was also analyzed using this method (p. 42).

An aliquot from the headspace at 1.5 hours (0.06 days) was also analyzed by HPLC (p. 28). However, the HPLC method was not specified.

Identification and quantification of transformation products: Transformation products were separated and quantified using HPLC as described for the parent compound (pp. 31, 40).

Table 6: Reference compounds available for identifying transformation products of chloropicrin.

Applicant codes	Chemical Name
Nitromethane	
Sodium bicarbonate	
Methanol	
1,3,5-Trioxane	1,3,5-Trioxane
2-Nitroethanol	2-Nitroethanol
Formaldehyde	

Data obtained from p. 24, Table I, p. 47 of the study report.

Detection limits (LOD, LOQ) for the parent compound and transformation products: For HPLC analyses, limits of detection (LOD) were reported as twice background (p. 32). The LSC LOD was 0.067 ppm. No other values were reported.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: The test conditions outlined in the study appear to have been maintained throughout the 54-day incubation. The systems were moderately reducing with redox potentials of -10 to +198 mV (Table VII, p. 53). In the water layer, dissolved oxygen was 0.23-1.63 (units not reported); pH levels were 6.6-7.9, with the exception of 8.1-8.7 at days 2 and 54 (one of two replicates).

B. MATERIAL BALANCE: Overall recovery of radiolabeled material averaged 98.2 ± 2.8% (range 91.4-103.0%) of the applied, with no pattern of decline in recoveries during the 54-day study (Table VI, p. 52). Following application of [^{14}C]chloropicrin to the water-soil systems, [^{14}C]residues partitioned from the water layer to the soil with average (n = 2) distribution soil:water ratios of 1:17 at time 0, 1:6 at 1 day, 1:1 at 12-26 days and was 2:1 at 54 days.

Table 7. Biotransformation of [^{14}C]chloropicrin, expressed as percentage of applied radioactivity (mean ± s.d., n = 2), in California deionized water-sandy loam soil under anaerobic conditions.

Compound		Sampling times (days)								
		0	**0.06**	**0.17**	**1**	**2**	**5**	**12**	**26**	**54**
Chloropicrin[1]	water	49.5 ± 59.7	26.7 ± 2.3	4.6 ± 3.7	0.8 ± 0.0	0.0, 1.1	ND	ND	0.0, 0.1	ND
	soil	0.0, 4.6	NA	ND	ND	ND	ND	ND	NA	NA
	volatile	NA	18.8 ± 1.2	6.7 ± 1.2	1.8	1.1	NA	NA	NA	NA
	system	51.8 ± 62.9	45.5 ± 1.1	11.2 ± 4.9	1.7 ± 1.3	1.1 ± 1.6	ND	ND	0.0, 0.1	ND
Chloronitro-methane	water	41.3 ± 55.2	ND	51.5 ± 6.7	ND	ND	ND	ND	0.2	0.0, 0.1
	soil	0.0, 0.4	NA	1.6 ± 0.3	ND	ND	0.1, 0.0	ND	NA	NA
	volatile	NA	0.4, 0.0	ND	0.1	ND	ND	NA	NA	NA
	system	41.5 ± 54.9	0.4, 0.0	53.1 ± 7.0	0.1	ND	0.1, 0.0	ND	0.2	0.0, 0.1
Nitromethane	water	ND	ND[2]	13.4 ± 0.1	53.4 ± 2.5	49.3 ± 5.7	47.3 ± 0.1	10.5 ± 1.2	16.9, 0.0	ND
	soil	1.4, 0.0	NA	1.7 ± 0.4	3.3 ± 0.4	2.9	3.0 ± 0.0	0.1	NA	NA
	volatile	NA	ND	ND	1.4	1.0	NA	NA	NA	NA
	system	1.4, 0.0	ND[2]	15.0 ± 0.4	57.4 ± 1.9	51.3 ± 7.0	50.3 ± 0.1	10.5 ± 1.1	16.9, 0.0	ND
Polar	water	ND	ND	ND	1.9, 0.0	3.1 ± 3.6	1.1 ± 0.4	11.1 ± 5.9	8.8 ± 4.5	13.0 ± 0.4
	soil	ND	NA	0.1, 0.0	0.1, 0.0	ND	ND	0.6 ± 0.6	NA	NA
	volatile	NA	0.1 ± 0.0	ND	ND	0.3	NA	NA	NA	NA
	system	ND	0.1 ± 0.0	0.1, 0.0	2.0, 0.0	3.2 ± 3.8	1.1 ± 0.4	11.6 ± 5.2	8.8 ± 4.5	13.0 ± 0.4
Unknown (Rt 9 min).	water	ND	ND[2]	7.3 ± 1.6	5.9 ± 0.5	6.8 ± 3.7	ND	ND	0.0, 0.3	ND
	soil	ND	NA	0.7 ± 0.5	0.5 ± 0.2	0.1	0.0, 0.1	NA	NA	NA
	system	ND	ND[2]	8.0 ± 2.1	6.3 ± 0.7	6.9 ± 3.6	0.0, 0.1	ND	0.0, 0.3	ND
KOH	CO_2	NA	NA	0.7, 0.0	1.2 ± 0.4	2.7 ± 1.7	1.1 ± 0.2	8.5 ± 8.4	1.9 ± 1.3	4.1 ± 0.4
	Volatiles	NA	NA	2.7 ± 0.1	13.6 ± 1.8	13.6 ± 8.6	28.4 ± 2.3	32.1 ± 4.5	47.8 ± 3.0	41.6 ± 3.0
	Total	NA	NA	3.0 ± 0.4	14.8 ± 1.4	16.3 ± 6.9	29.5 ± 2.1	40.6 ± 3.9	49.6 ± 1.7	45.7 ± 3.5
Volatile organics		1.1 ± 0.3	8.8 ± 1.8	8.4 ± 1.6	4.9 ± 0.1	2.4 ± 0.7	2.7 ± 0.5	0.7 ± 0.5	2.5 ± 0.3	0.6 ± 0.1
Headspace volatiles		NA	10.9 ± 0.4	4.0 ± 1.1	0.4 ± 0.2	0.7 ± 0.4	0.4 ± 0.1	0.3 ± 0.2	0.1 ± 0.0	0.1, 0.0

Extractable sediment residues		4.3 ± 1.2	NA	4.3 ± 0.3	4.1 ± 0.5	2.9 ± 0.1	3.2 ± 0.1	1.3 ± 0.2	1.3 ± 0.1	1.9 ± 0.3
Nonextractable sediment residues		1.2 ± 1.0	2.5 ± 0.1	3.7 ± 1.3	6.8 ± 0.4	11.0 ± 2.3	13.7 ± 1.1	26.3 ± 5.4	22.3 ± 5.0	32.0 ± 6.4
Total recovery	water	93.5 ± 2.3	77.7 ± 4.0	79.0 ± 1.3	62.2 ± 3.9	65.7 ± 6.9	48.8 ± 0.6	27.4 ± 2.6	21.7 ± 1.6	17.8 ± 2.2
	soil	5.5 ± 0.2	2.5 ± 0.1	8.0 ± 1.0	10.9 ± 0.1	13.9 ± 2.4	16.8 ± 1.0	27.6 ± 5.6	23.5 ± 4.9	33.9 ± 6.2
	system	100.0 ± 2.8	100.1 ± 2.5	102.4 ± 0.9	93.0 ± 2.3	99.0 ± 1.2	98.1 ± 0.1	96.4 ± 0.6	97.4 ± 1.9	97.9 ± 0.5

1 Reviewer's Comment No. 2.
2 Poor resolution did not allow for quantitation.
ND = 0.0
NA = Not analyzed.
Data obtained from Table VI, p. 52, Tables IX-XI, pp. 55-57 and Table XIII, p. 59 in the study report.

C. TRANSFORMATION OF PARENT COMPOUND: [^{14}C]Chloropicrin dissipated rapidly in the total system decreasing from 96.3% (one replicate) of the applied at time 0 to an average of 45.5% at 1.5 hours (0.06 days) days to 1.1% at 2 days, was not detected from 5 to 12 days, and was last detected at 0.1% (one replicate) at 26 days posttreatment (DER Attachment 2). In the water layer, [^{14}C]chloropicrin decreased from 91.7% at day 0 to 26.7% at 1.5 hours (0.06 days) days to 0.6% at 2 days, was not detected from 5 to 12 days, and was last detected at 0.1% (one replicate) at 26 days posttreatment. In the soil, [^{14}C]chloropicrin was detected in a single replicate; 4.6% of the applied at time 0.

HALF-LIFE/DT50/DT90: Observed DT50 values of chloropicrin were <1.5 hours in the water layer and total system. Based on first order linear regression analysis (Excel 2000, 0-2 days), the half-lives of chloropicrin were 0.4 days in the water layer and total system (DER Attachment 2). Based on nonlinear analysis (SigmaPlot v 9), half-lives were 0.03 days in the water and total system. A half-life in soil could not be calculated because it was detected in a single replicate at time 0. Using the data through four hours, the study authors determined a half-life for [^{14}C]chloropicrin of 1.3 hours (r^2 = 1.0; figures 55-56, pp. 159-160).

The Chloropicrin Manufacturers' Task Force submitted comments to EPA regarding the Phase 3 Risk Assessment for Chloropicrin (February 28, 2007). In these comments, the Task Force cites that EPA calculated an anaerobic aquatic metabolism half-life of 0.05 days (methods not described) for chloropicrin (p. 29 of *Comments on USEPA's Chloropicrin Risk Assessment Phase 3*).

Half-lives/DT50/DT90

Phase	Half-life/DT50 [1] (days)	First order linear regression equation	r^2	DT50[2] (hours)	DT90
Deionized water					
Linear/natural log	0.4	y = -1.6578x + 2.6732	0.5609	--	--
Nonlinear/normal	0.03	--	0.9972	--	--
Observed DT50	<0.06	--	--	--	--
Sandy loam soil					
Linear/natural log	ND	--	--	--	--
Nonlinear/normal	ND	--	--	--	--
Observed DT50	ND	--	--	--	--
Total system					
Linear/natural log	0.4	y = -1.6643x + 2.6833	0.559	--	--
Nonlinear/normal	0.03	--	0.9973	1.3	--
Observed DT50	<0.06	--	--	--	--

1 Determined by the primary reviewer using Excel 2000 (linear) and Sigmaplot v 9.0 (nonlinear) and individual sample data obtained from Tables IX-X, pp. 55-56 of the study report (DER Attachment 2).
2 Determined by the study author (Figures 55-56, pp. 159-160).
ND Not determined.

TRANSFORMATION PRODUCTS: Two major transformation products were isolated and no minor products were identified (Tables IX-X, pp. 55-56). Nitromethane increased to maximum average of 57.4% of the applied at 1 day and was last detected at 16.9% (one replicate) at 26 days. In water, nitromethane was a maximum average 53.4% of the applied at 1 days and was last detected at 16.9% (one replicate) at 26 days. In soil nitromethane was a maximum average 3.3% at 1 day. Volatile nitromethane was a maximum 1.4%. Chloronitromethane increased to a maximum average of 53.1% (51.5% in water, 1.6% in soil) of the applied at 4 hours (0.17 days) and was <0.2% thereafter. Unidentified polar [^{14}C]residues were detected at maximum averages of 13.0%, 0.6%, 13.0% and 0.3% of the applied in the water, soil, total system and volatiles, respectively. An unknown with an Rt of 9 minutes was a maximum 7.3%, 0.7% and 8.0% of the applied in the water layer, soil and total system, respectively.

NONEXTRACTABLE AND EXTRACTABLE RESIDUES: Extractable soil [^{14}C]residues were 4.1-4.3% of the applied at 0-1 day and were 1.3-2.9% thereafter. Nonextractable soil [^{14}C]residues increased from 1.2% of applied at time 0 posttreatment to 32.0 at 54 days (Table VI, p. 52, DER Attachment 2). At study termination, organic matter fractionation of nonextractable [^{14}C]residues found 24.4% and 1.3% of the applied radioactivity associated with the fulvic acids and humic acids, respectively (Table XII, p. 58).

VOLATILIZATION: The maximum level of volatilized $^{14}CO_2$ detected at any sampling interval was 14.4% of the applied (Table XIII, p. 59). Other volatiles trapped in the KOH solution were a maximum average 47.8% at 26 days. Volatile [^{14}C]organic compounds from the polyurethane foam

were a maximum 8.8% at 1.5 hours (0.06 days, Table VI, p. 52). At 1.5 hours 6.8-9.3% was identified as volatile chloropicrin in the polyurethane foam (Table XIV, p. 60). Volatiles in the headspace were a maximum average 10.9% at 1.5 hours. At 1.5 hours 10.3-11.1% was identified as volatile chloropicrin in headspace (Table XI, p. 57).

TRANSFORMATION PATHWAY: A transformation pathway was provided (Figure 5, p. 67). Chloropicrin degraded rapidly into dichloronitromethane which further degraded to nitromethane. Nitromethane was involved the formation of bound soil residues and mineralization to CO_2.

Table 8: Chemical names and CAS numbers for the transformation products of chloropicrin.

Applicants Code Name	CAS Number	Chemical Name	Chemical Formula	MW (g/mol)	Smiles String
Nitromethane					
Chloronitromethane					

D. SUPPLEMENTARY EXPERIMENT-RESULTS: The results from the supplementary samples at time 0 and 4 hours were incorporated into the definitive study results.

III. STUDY DEFICIENCIES

No significant deviations from good scientific practices or Subdivision N guidelines were noted.

IV. REVIEWER'S COMMENTS

1. The study authors reported that a second set of samples (time 0 and 4-hour) were prepared and incubated in order to establish the degradation of the parent compound (p. 21). The half-life calculation of the parent is of questionable validity since time 0 and 4-hour samples were not treated at the same time as the other samples (p. 43). Sound scientific practice dictates that the test samples be treated with the same dosing solution and incubated simultaneously to ensure similar treatment rates and similar testing conditions. It is important that the time 0 data point be determined accurately. In addition, a minimum of four data points are needed for a valid calculation of a half-life. However, due to rapid dissipation of the parent compound, an additional study may not provide new useful information.

2. It is not clear why the supplemental samples from time 0 vary so greatly. In one replicate, chloropicrin accounts for 91.7% of the applied in water and 7.3% in the second replicate (Table IX, p. 55). Chloronitromethane accounts for 2.3% of the applied and 80.3% in the corresponding replicates. The reviewer considered the second replicate an outlier and did not use it for half-life calculations.

3. Purified, deionized water, rather than natural water was utilized to flood the soil samples (p. 26). Subdivision N Guidelines require that the test water used to flood the soil be representative of the intended use site.

4. The analytical methods were inadequate for the characterization of the residues in water samples removed at later sampling intervals. The HPLC column recoveries for the water phase samples were 103-104% at 0-1.5 hours posttreatment, decreased to 83.6% by 5 days and were 24.1% at 54 days (Table IX, p. 55). The study authors did not provide an explanation for this decrease. Clarification of the data presented in Table IX (p. 55) may be necessary.

5. The data from the microbial analyses indicated that the soil was viable throughout the incubation period (Table III, p. 49). However, the study authors stated that there was a one hundred-fold decrease in colony forming units over the course of the study (p. 35). The study authors stated that this decrease may have been due to the bactericidal properties of chloropicrin.

6. The dissolved oxygen content of one of the two replicates at 5 days posttreatment was an outlier and was not included in this report (Table VII, p. 53). The study authors stated that this value (4.3) "may be high due to incomplete displacement of air in the sampling vial" (p. 53). Units of concentration were not reported for the dissolved oxygen content data.

7. Evolved $^{14}CO_2$ accounted for ≤8.5% of the applied radioactivity detected in the KOH traps (p. 38, Table XIII, p. 59). The study authors stated that the remaining [^{14}C]residues (formaldehyde, methanol and 1,3,5-trioxane)were chemically formed by volatilization of the transformation product nitromethane followed by adsorption and reaction with KOH (pp. 41-42).

8. The residue data were reported as percentages of the applied radioactivity. In future studies submitted to EPA, it is necessary that residue data also be submitted in units of concentration, such as ppm.

9. The study authors stated that the headspace analysis was not conducted for the time 0 and 4-hour samples so that the water phase could be analyzed immediately after treatment (p. 29).

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 162-3, Anaerobic Aquatic Metabolism Studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.

2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.

3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

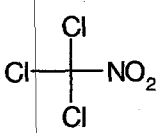
4. Wolfe, N., *et al.* 1990. Abiotic transformations in water, sediments and soil. *In* Pesticides in the Soil Environment, Soil Science Society of America, pp. 103-110.

Attachment 1: Structures of Parent Compound and Transformation Products

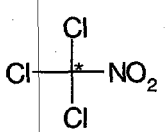
Chloropicrin

IUPAC Name: Trichloronitromethane.
CAS Name: Trichloronitromethane.
CAS Number: 76-06-2.
SMILES String: O=N(=O)C(Cl)(Cl)Cl (EPI Suite, v3.12 SMILES).

Unlabeled



[^{14}C]Chloropicrin

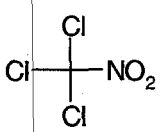


* = Location of the radiolabel.

Identified Compounds

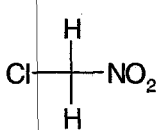
Chloropicrin

IUPAC Name: Trichloronitromethane.
CAS Name: Trichloronitromethane.
CAS Number: 76-06-2.
SMILES String: O=N(=O)C(Cl)(Cl)Cl (EPI Suite, v3.12 SMILES).



Chloronitromethane

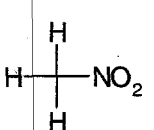
IUPAC Name: Chloro(nitro)methane.
CAS Name: Not reported.
CAS Number: Not reported.



Structure created by reviewer.

Nitromethane

IUPAC Name: Nitromethane.
CAS Name: Not reported.
CAS Number: Not reported.



Carbon Dioxide

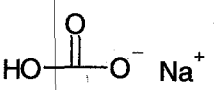
IUPAC Name: Not reported.
CAS Name: Not reported.
CAS Number: Not reported.

O=C=O

Unidentified Reference Compounds

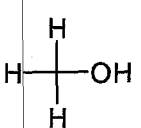
Sodium bicarbonate

IUPAC Name: Sodium hydrogen carbonate.
CAS Name: Not reported.
CAS Number: Not reported.

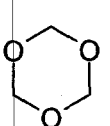


Methanol

IUPAC Name: Methanol.
CAS Name: Not reported.
CAS Number: Not reported.

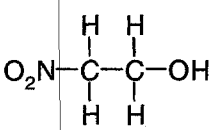


1,3,5 Trioxane
IUPAC Name: 1,3,5-Trioxane.
CAS Name: Not reported.
CAS Number: Not reported.



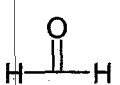
2 Nitroethanol

IUPAC Name: 2-Nitroethanol.
CAS Name: Not reported.
CAS Number: Not reported.



Formaldehyde

IUPAC Name: Formaldehyde.
CAS Name: Not reported.
CAS Number: Not reported.



Attachment 2. Excel and SigmaPlot Spreadsheets

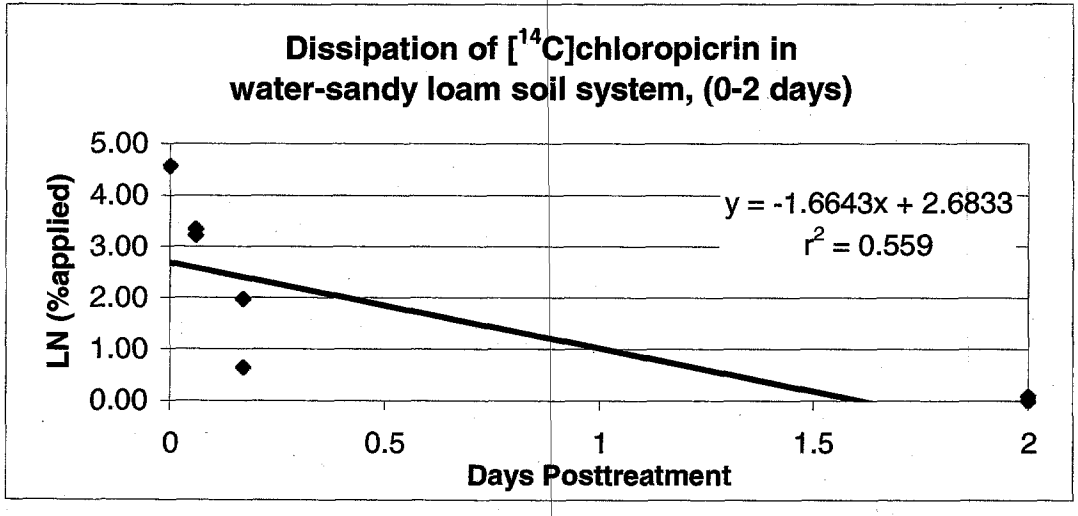
Chemical: Chloropicrin
MRID: 43759301
PC: 081501
Guideline: 162-3

Total system

Half-life (days): 0.4

Days Posttreatment	Chloropicrin % of applied	ln % applied
0	96.3	4.5675
0.06	28.3	3.3429
0.06	25.1	3.2229
0.17	7.2	1.9741
0.17	1.9	0.6419
1	0.8	-0.2231
1	0.8	-0.2231
2	0.0	#NUM!
2	1.1	0.0953

Data obtained from Table IX-X, pp. 55-56 in the study report and calculated.
Replicate two from time 0 was considered an outlier.



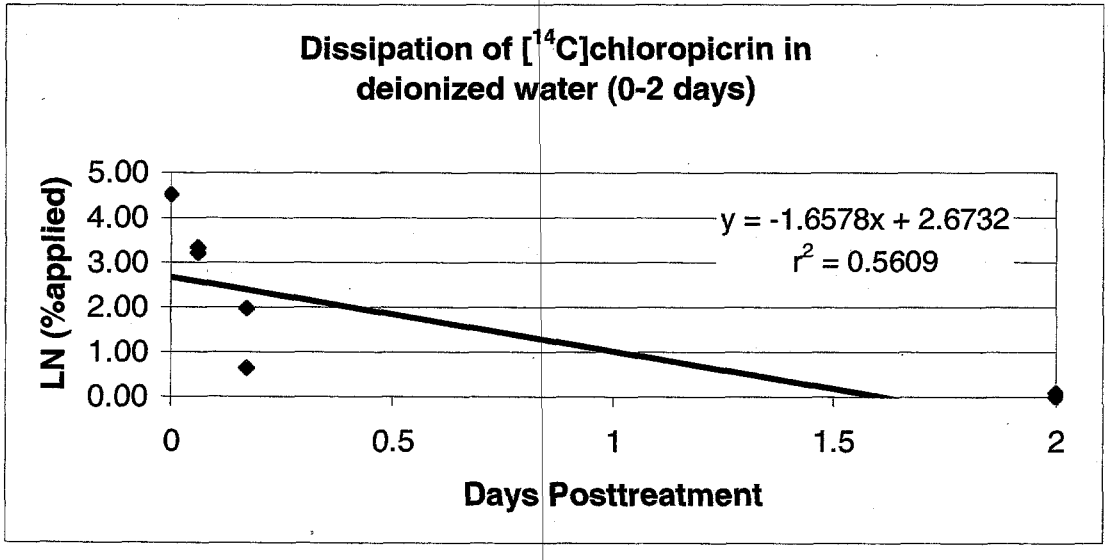
Chemical: Chloropicrin
MRID: 43759301
PC: 081501
Guideline: 162-3

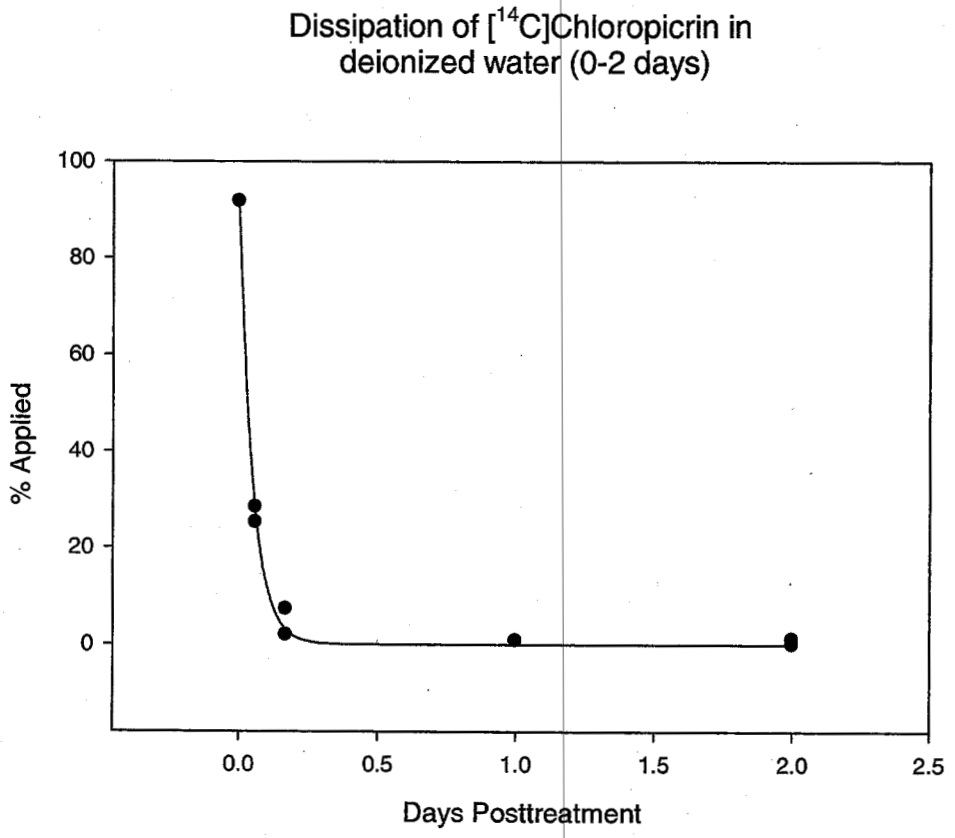
Water

Half-life (days): 0.4

Days Posttreatment	Chloropicrin % of applied	ln % applied
0	91.7	4.5185
0.06	28.3	3.3429
0.06	25.1	3.2229
0.17	7.2	1.9741
0.17	1.9	0.6419
1	0.8	-0.2231
1	0.8	-0.2231
2	0.0	#NUM!
2	1.1	0.0953

Data obtained from Table IX, p. 55 in the study report and calculated.
Replicate two from time 0 was considered an outlier.




Dissipation of [14C]Chloropicrin in deionized water (0-2 days)
% Applied
100
80
60
40
20
0
0.0
0.5
1.0
1.5
2.0
2.5
Days Posttreatment

Dissipation of [14C]Chloropicrin in deionized water (0-2 days)
Nonlinear Regression

Data Source: Data 1 in Notebook2
Equation: Single, 2 Parameter

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9986	0.9972	0.9964	1.9772

	Coefficient	Std. Error	t	P	VIF
a	91.5103	1.9709	46.4297	<0.0001	1.1712
b	20.2247	0.8867	22.8091	<0.0001	1.1712

Analysis of Variance:

	DF	SS	MS
Regression	2	9870.3652	4935.1826
Residual	7	27.3648	3.9093
Total	9	9897.7300	1099.7478

Statistical Tests:

PRESS 948.7563

Durbin-Watson Statistic 3.0979 Failed

Normality Test Passed (P = 0.4255)

K-S Statistic = 0.2778 Significance Level = 0.4255

Constant Variance Test Passed (P = 0.3811)

Power of performed test with alpha = 0.0500: 1.0000

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	91.5103	0.1897	0.0959	1.2085	1.2578
2	27.1933	1.1067	0.5598	0.7599	0.7345
3	27.1933	-2.0933	-1.0587	-1.4372	-1.5849
4	2.9395	4.2605	2.1548	2.2059<	3.6987<
5	2.9395	-1.0395	-0.5258	-0.5382	-0.5089
6	1.5066E-007	0.8000	0.4046	0.4046	0.3791
7	1.5066E-007	0.8000	0.4046	0.4046	0.3791
8	2.4803E-016	-2.4803E-016	-1.2545E-016	-1.2545E-016	-1.1614E-016
9	2.4803E-016	1.1000	0.5563	0.5563	0.5269

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	115.1617<	0.9937	15.7947<

2	0.2434	0.4574	0.6743
3	0.8706	0.4574	-1.4551
4	0.1167	0.0458	0.8100
5	0.0069	0.0458	-0.1115
6	3.6695E-016	4.4828E-015	2.5379E-008
7	3.6695E-016	4.4828E-015	2.5379E-008
8	3.8585E-064	4.9038E-032	-2.5719E-032
9	7.5892E-033	4.9038E-032	1.1667E-016

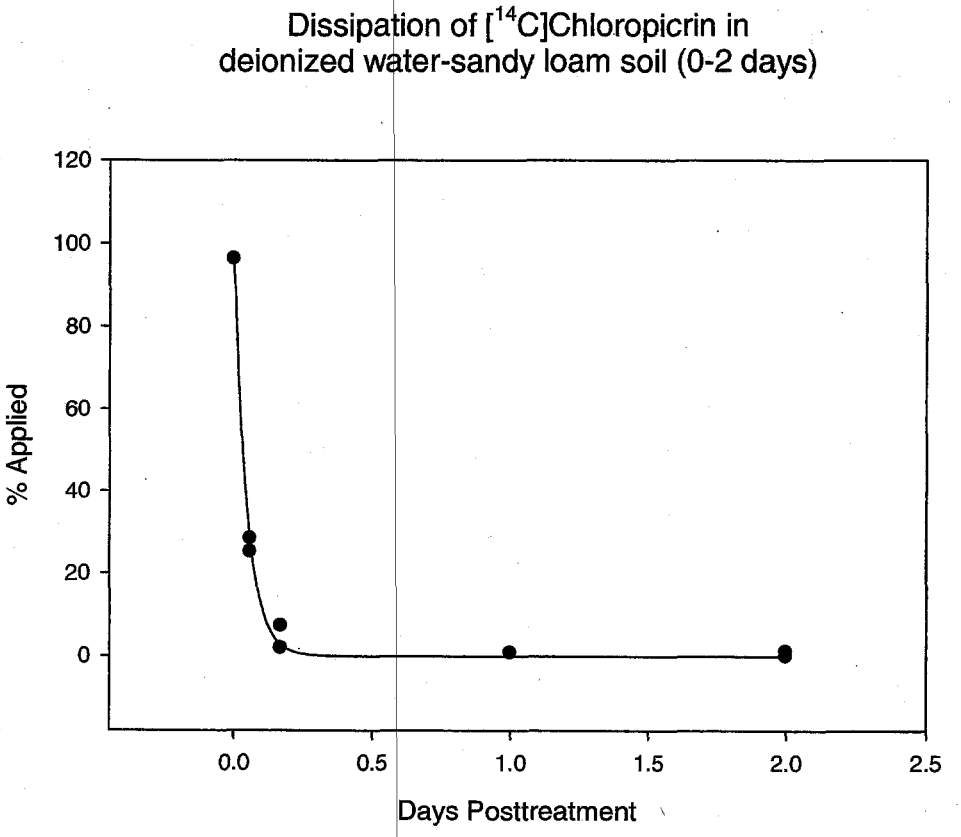
95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	91.5103	86.8498	96.1709	84.9089	98.1118
2	27.1933	24.0313	30.3552	21.5491	32.8374
3	27.1933	24.0313	30.3552	21.5491	32.8374
4	2.9395	1.9394	3.9397	-1.8415	7.7206
5	2.9395	1.9394	3.9397	-1.8415	7.7206
6	1.5066E-007	-1.6237E-007	4.6368E-007	-4.6753	4.6753
7	1.5066E-007	-1.6237E-007	4.6368E-007	-4.6753	4.6753
8	2.4803E-016	-7.8730E-016	1.2834E-015	-4.6753	4.6753
9	2.4803E-016	-7.8730E-016	1.2834E-015	-4.6753	4.6753

Fit Equation Description:

[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)
asign(q)=if(mean(q)>=0,1,-1)
[Parameters]
a = if(F(0)[1]< 307, if(F(0)[1]>-307, asign(y)*10^F(0)[1], asign(y)*10^(-307)), asign(y)*10^307) "Auto {{previous: 91.5103}}
b = if(x50(x,y)-min(x)=0, 1, -ln(.5)/(x50(x,y)-min(x))) "Auto {{previous: 20.2247}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance = 1e-10
stepsize = 1
iterations=200

Number of Iterations Performed = 8


Dissipation of [14C]Chloropicrin in
deionized water-sandy loam soil (0-2 days)
% Applied
120
100
80
60
40
20
0
0.0
0.5
1.0
1.5
2.0
2.5
Days Posttreatment

Dissipation of [14C]Chloropicrin in
deionized water-sandy loam soil (0-2 days)
Nonlinear Regression

Data Source: Data 1 in Notebook1
Equation: Single, 2 Parameter

R	Rsqr	Adj Rsqr	Standard Error of Estimate
0.9986	0.9973	0.9965	2.0396

	Coefficient	Std. Error	t	P	VIF
a	96.1093	2.0346	47.2372	<0.0001	1.1563
b	21.0253	0.9143	22.9964	<0.0001	1.1563

Analysis of Variance:

	DF	SS	MS
Regression	2	10733.4106	5366.7053
Residual	7	29.1194	4.1599
Total	9	10762.5300	1195.8367

Statistical Tests:

PRESS 1576.2209

Durbin-Watson Statistic 3.0020 Failed

Normality Test Passed (P = 0.4255)

K-S Statistic = 0.2778 Significance Level = 0.4255

Constant Variance Test Passed (P = 0.6758)

Power of performed test with alpha = 0.0500: 1.0000

Regression Diagnostics:

Row	Predicted	Residual	Std. Res.	Stud. Res.	Stud. Del. Res.
1	96.1093	0.1907	0.0935	1.3395	1.4381
2	27.2204	1.0796	0.5293	0.7228	0.6956
3	27.2204	-2.1204	-1.0396	-1.4197	-1.5576
4	2.6944	4.5056	2.2091	2.2531<	3.9794<
5	2.6944	-0.7944	-0.3895	-0.3973	-0.3720
6	7.1054E-008	0.8000	0.3922	0.3922	0.3672
7	7.1054E-008	0.8000	0.3922	0.3922	0.3672
8	5.2531E-017	-5.2531E-017	-2.5756E-017	-2.5756E-017	-2.3845E-017
9	5.2531E-017	1.1000	0.5393	0.5393	0.5100

Influence Diagnostics:

Row	Cook's Dist	Leverage	DFFITS
1	183.1684<	0.9951	20.5484<

2	0.2259	0.4637	0.6469
3	0.8713	0.4637	-1.4483
4	0.1022	0.0387	0.7987
5	0.0032	0.0387	-0.0747
6	7.6755E-017	9.9779E-016	1.1599E-008
7	7.6755E-017	9.9779E-016	1.1599E-008
8	7.2951E-067	2.1995E-033	-1.1183E-033
9	3.1988E-034	2.1995E-033	2.3919E-017

95% Confidence:

Row	Predicted	Regr. 5%	Regr. 95%	Pop. 5%	Pop. 95%
1	96.1093	91.2982	100.9203	89.2970	102.9215
2	27.2204	23.9362	30.5046	21.3855	33.0553
3	27.2204	23.9362	30.5046	21.3855	33.0553
4	2.6944	1.7454	3.6434	-2.2209	7.6098
5	2.6944	1.7454	3.6434	-2.2209	7.6098
6	7.1054E-008	-8.1289E-008	2.2340E-007	-4.8229	4.8229
7	7.1054E-008	-8.1289E-008	2.2340E-007	-4.8229	4.8229
8	5.2531E-017	-1.7365E-016	2.7871E-016	-4.8229	4.8229
9	5.2531E-017	-1.7365E-016	2.7871E-016	-4.8229	4.8229

Fit Equation Description:

```
[Variables]
x = col(1)
y = col(2)
reciprocal_y = 1/abs(y)
reciprocal_ysquare = 1/y^2
'Automatic Initial Parameter Estimate Functions
F(q)=if(size(x)>1, if(total(abs(y))>0, ape(x,log(abs(y)),1,0,1), -306), 0)
asign(q)=if(mean(q)>=0,1,-1)
[Parameters]
a = if(F(0)[1]< 307, if(F(0)[1]>-307, asign(y)*10^F(0)[1], asign(y)*10^(-307)), asign(y)*10^307) "Auto {{previous: 96.1093}}
b = if(x50(x,y)-min(x)=0, 1,  -ln(.5)/(x50(x,y)-min(x)))  "Auto {{previous: 21.0253}}
[Equation]
f = a*exp(-b*x)
fit f to y
"fit f to y with weight reciprocal_y
"fit f to y with weight reciprocal_ysquare
[Constraints]
b>0
[Options]
tolerance = 1e-10
stepsize = 1
iterations=200
```

Number of Iterations Performed = 8

Chemical: Chloropicrin									
MRID: 43759301									
PC: 081501									
Guideline: 162-3									
HPLC Distribution									
Days	Chloropicrin				Chloronitromethane				
Posttreatment	% Applied				% Applied				
	water	soil	volatile	system	water	soil	volatile	system	
0	7.3			7.3	80.3			80.3	
0	91.7	4.6		96.3	2.3	0.4		2.7	
average	49.5	4.6		51.8	41.3			41.5	
sd	59.7			62.9	55.2			54.9	
0.06	28.3		17.9	46.2			0.4	0.4	
0.06	25.1		19.6	44.7					
average	26.7		18.8	45.5					
sd	2.3		1.2	1.1					
0.17	7.2		7.5	14.7	46.7	1.4		48.1	
0.17	1.9		5.8	7.7	56.2	1.8		58	
average	4.6		6.7	11.2	51.5	1.6		53.1	
sd	3.7		1.2	4.9	6.7	0.3		7.0	
1	0.8		0.0	0.8			0	0	
1	0.8		1.8	2.6			0.1	0.1	
average	0.8			1.7					
sd	0.0			1.3					
2	0.0		0.0	0.0					
2	1.1		1.1	2.2					
average	0.6			1.1					
sd	0.8			1.6					
5						0.1		0.1	
5									
average									
sd									
12									
12									
average									
sd									
26	0.0			0.0	0.2			0.2	
26	0.1			0.1					
average									
sd									

54					0				
54					0.1			0.1	
average									
sd									
Data obtained from Tables IX-XI, pp. 55-57 in the study report.									
Volatile was calculated by adding headspace and PUF extract.									
Chemical: Chloropicrin									
MRID: 43759301									
PC: 081501									
Guideline: 162-3									
HPLC Distribution									
Days	Nitromethane				Polar				
Posttreatment	% Applied				% Applied				
	water	soil	volatile	system	water	soil	volatile	system	
0		1.4		1.4					
0									
average		1.4							
sd									
0.06							0.1		
0.06							0.1		
average									
sd									
0.17	13.4	1.9		15.3		0.1			
0.17	13.3	1.4		14.7		0			
average	13.4	1.7		15.0					
sd	0.1	0.4		0.4					
1	55.2	3.5	0.0	58.7	1.9	0.1		2	
1	51.6	3.0	1.4	56.0	0				
average	53.4	3.3		57.4					
sd	2.5	0.4		1.9					
2	53.3	2.9	0.0	56.2	0.5		0	0.8	
2	45.3		1.0	46.3	5.6		0.3	5.6	
average	49.3			51.3	3.1			3.2	
sd	5.7			7.0	3.6			3.4	
5	47.4	3.0		50.4	1.3			1.3	
5	47.2	3.0		50.2	0.8			0.8	

average	47.3	3.0		50.3	1.1			1.1	
sd	0.1	0.0		0.1	0.4			0.4	
12	11.3	0.0		11.3	15.2	0.1		15.3	
12	9.6	0.1		9.7	6.9	1.0		7.9	
average	10.5			10.5	11.1	0.6		11.6	
sd	1.2			1.1	5.9	0.6		5.2	
26	16.9			16.9	5.6			5.6	
26	0.0			0.0	12			12	
average					8.8			8.8	
sd					4.5			4.5	
54					13.3			13.3	
54					12.7			12.7	
average					13.0			13.0	
sd					0.4			0.4	
Data obtained from Tables IX-XI, pp. 55-57 in the study report.									
Volatile was calculated by adding headspace and PUF extract.									
Chemical: Chloropicrin									
MRID: 43759301									
PC: 081501									
Guideline: 162-3									
HPLC Distribution									

Days	Unk			CO_2	Volatile	Total	Volatiles		
Posttreatment	% Applied			% Applied			% Applied		
	Water	soil	system	KOH			Puf extract	Puf	Total
0							0.4	0.5	0.9
0							1.2	0.1	1.3
average							0.8	0.3	1.1
sd							0.6	0.3	0.3
0.06							7.4	0.1	7.5
0.06							9.6	0.5	10.1
average							8.5	0.3	8.8
sd							1.6	0.3	1.8
0.17	8.4	1	9.4	0.7	2.6	3.3	8.8	0.7	9.5
0.17	6.2	0.3	6.5	0	2.7	2.7	6.5	0.7	7.2
average	7.3	0.7	8.0		2.7	3.0	7.7	0.7	8.4

sd	1.6	0.5	2.1		0.1	0.4	1.6	0.0	1.6
1	5.5	0.3	5.8	1.5	12.3	13.8	1.9	2.9	4.8
1	6.2	0.6	6.8	0.9	14.9	15.8	3.4	1.5	4.9
average	5.9	0.5	6.3	1.2	13.6	14.8	2.7	2.2	4.9
sd	0.5	0.2	0.7	0.4	1.8	1.4	1.1	1.0	0.1
2	4.2	0.1	4.3	1.5	19.6	21.1	1.3	0.6	1.9
2	9.4		9.4	3.9	7.5	11.4	2.8	0.1	2.9
average	6.8		6.9	2.7	13.6	16.3	2.1	0.4	2.4
sd	3.7		3.6	1.7	8.6	6.9	1.1	0.4	0.7
5		0	0	1.2	26.8	28	2.0	1.0	3.0
5		0.1	0.1	0.9	30	30.9	1.2	1.1	2.3
average			0.1	1.1	28.4	29.5	1.6	1.1	2.7
sd			0.1	0.2	2.3	2.1	0.6	0.1	0.5
12				14.4	28.9	43.3	0.1	0.2	0.3
12				2.5	35.3	37.8	0.2	0.8	1.0
average				8.5	32.1	40.6	0.2	0.5	0.7
sd				8.4	4.5	3.9	0.1	0.4	0.5
26	0			0.9	49.9	50.8	0.9	1.4	2.3
26	0.3			2.8	45.6	48.4	0.9	1.8	2.7
average				1.9	47.8	49.6	0.9	1.6	2.5
sd				1.3	3.0	1.7	0.0	0.3	0.3
54				3.8	39.4	43.2	0.1	0.4	0.5
54				4.4	43.7	48.1	0.1	0.5	0.6
average				4.1	41.6	45.7	0.1	0.5	0.6
sd				0.4	3.0	3.5	0.0	0.1	0.1

Data obtained from Table VI, p. 52, Tables IX-XI, pp. 55-57, Table XIII, p. 59 in the study report.

KOH volatiles was calculated by subtracting CO_2 values from total.

Chemical: Chloropicrin

MRID: 43759301

PC: 081501

Guideline: 162-3

HPLC Distribution

Days	Headspace	Extract	Nonextract	Soil	Water	Recovery
Posttreatment	% Applied					
0		3.4	1.9	5.3	91.8	98.0
0		5.1	0.5	5.6	95.1	102.0
average		4.3	1.2	5.5	93.5	100.0

sd		1.2	1.0	0.2	2.3	2.8			
0.06	11.2		2.5	2.5	80.5	101.8			
0.06	10.6		2.4	2.4	74.9	98.3			
average	10.9		2.5	2.5	77.7	100.1			
sd	0.4		0.1	0.1	4.0	2.5			
0.17	4.8	4.5	2.8	7.3	78.1	103.0			
0.17	3.2	4.1	4.6	8.7	79.9	101.7			
average	4.0	4.3	3.7	8.0	79.0	102.4			
sd	1.1	0.3	1.3	1.0	1.3	0.9			
1	0.2	4.4	6.5	10.9	64.9	94.6			
1	0.5	3.7	7.1	10.8	59.4	91.4			
average	0.4	4.1	6.8	10.9	62.2	93.0			
sd	0.2	0.5	0.4	0.1	3.9	2.3			
2	0.4	3.0	12.6	15.6	60.8	99.8			
2	1.0	2.8	9.4	12.2	70.6	98.1			
average	0.7	2.9	11.0	13.9	65.7	99.0			
sd	0.4	0.1	2.3	2.4	6.9	1.2			
5	0.4	3.1	14.4	17.5	49.2	98.1			
5	0.3	3.2	12.9	16.1	48.4	98.0			
average	0.4	3.2	13.7	16.8	48.8	98.1			
sd	0.1	0.1	1.1	1.0	0.6	0.1			
12	0.4	1.1	22.5	23.6	29.2	96.8			
12	0.1	1.4	30.1	31.5	25.5	95.9			
average	0.3	1.3	26.3	27.6	27.4	96.4			
sd	0.2	0.2	5.4	5.6	2.6	0.6			
26	0.1	1.3	18.7	20.0	22.8	96			
26	0.1	1.2	25.8	27.0	20.5	98.7			
average	0.1	1.3	22.3	23.5	21.7	97.4			
sd	0.0	0.1	5.0	4.9	1.6	1.9			
54	0.1	1.7	36.5	38.2	16.2	98.2			
54		2.1	27.4	29.5	19.3	97.5			
average		1.9	32.0	33.9	17.8	97.9			
sd		0.3	6.4	6.2	2.2	0.5			
Data obtained from Table VI, p. 52 in the study report.									

Attachement 3: Tansformation Pathway presented by Registrant
Illustration of Test System

Pages 42-43 - Access to registrant submitted data is restricted under FIFRA section 10(g)